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*Crystallographic report*

# A double chain coordination polymer: $\{[Zn(H_2O)_6][Zn(3,3',4,4'\text{-benzophenonetetracarboxylate})H_2O]\cdot 4H_2O\}_n$

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**The double-chain coordination polymer, $\{[Zn(H_2O)_6][Zn(bbtc)H_2O]\cdot 4H_2O\}_n$ (bbtc = 3, 3′, 4, 4′-benzophenonetetracarboxylate), features two kinds of zinc center. One is octahedrally coordinated by six aqua ligands and the other is coordinated by four carboxylate oxygen atoms, derived from three bbtc ligands, and a water molecule, forming a geometry intermediate between square-pyramidal and trigonal bipyramidal. Copyright © 2003 John Wiley & Sons, Ltd.**

**KEYWORDS:** zinc complex; benzophenonetetracarboxylic acid; crystal structure; coordination polymer

## COMMENT

Recently, $d^{10}$ metals have attracted considerable attention owing to their potential in optical applications.[1,2] In this context, we report the synthesis and crystal structure of a double-chain coordination polymer, namely $\{[Zn(H_2O)_6][Zn(bbtc)H_2O]\cdot 4H_2O\}_n$ (bbtc = 3, 3′, 4, 4′-benzophenonetetracarboxylate). There are two distinct zinc centers in the structure. As shown in Fig. 1, Zn2 is part of a discrete mononuclear entity and is coordinated by six aqua ligands in a nearly octahedral environment. Besides a water molecule, Zn1 is coordinated by four carboxylic oxygen atoms derived from three bbtc ligands. The Zn1 atom is in a severely distorted geometry that is intermediate between square-pyramidal and trigonal bipyramidal, with a small bias towards the latter. From the connectivity involving the Zn1 atoms and bbtc ligands, a double-chain of Zn-bbtc is generated (Fig. 2). Both the coordinating and lattice water molecules participate in hydrogen bonding to the carboxylic acid groups, resulting in a three-dimensional network structure.

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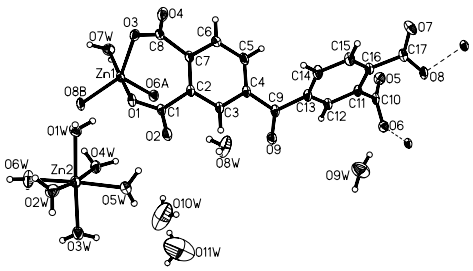


**Figure 1.** The crystallographic asymmetric unit of $\{[Zn(H_2O)_6][Zn(bbtc)H_2O]\cdot 4H_2O\}_n$ showing the atomic numbering scheme. Key geometric parameters: Zn1–O1 2.110(2), Zn1–O3 2.027(2), Zn1–O6A 2.002(2), Zn1–O8B 2.024(2), Zn1–O7W 2.137(3), Zn2–O1W 2.073(2), Zn2–O2W 2.114(3), Zn2–O3W 2.079(3), Zn2–O4W 2.218(2), Zn2–O5W 2.072(3), Zn2–O6W 2.051(3) Å; O1–Zn1–O3 85.0(1), O1–Zn1–O6A 100.0(1), O1–Zn1–O8B 90.9(1), O1–Zn1–O7W 173.0(1), O3–Zn1–O6A 113.9(1), O3–Zn1–O7W 88.7(1), O3–Zn1–O8B 139.6(1), O6A–Zn1–O8B 106.4(1), O6A–Zn1–O7W 85.3(1), O8B–Zn1–O7W 92.0(1), O1W–Zn2–O2W 86.7(1), O1W–Zn2–O4W 86.4(1), O1W–Zn2–O3W 176.4(1), O1W–Zn2–O5W 92.1(1), O1W–Zn2–O6W 92.2(1), O2W–Zn2–O3W 92.1(1), O2W–Zn2–O4W 172.8(1), O2W–Zn2–O5W 93.0(1), O2W–Zn2–O6W 91.6(1), O3W–Zn2–O4W 94.9(1), O3W–Zn2–O5W 84.6(1), O3W–Zn2–O6W 91.2(1), O4W–Zn2–O5W 89.4(1), O4W–Zn2–O6W 86.5(1), O6W–Zn2–O5W 173.9(1)°. Symmetry code: A = $1-x, 2-y, -z$; B = $x, y-1, 1+z$.

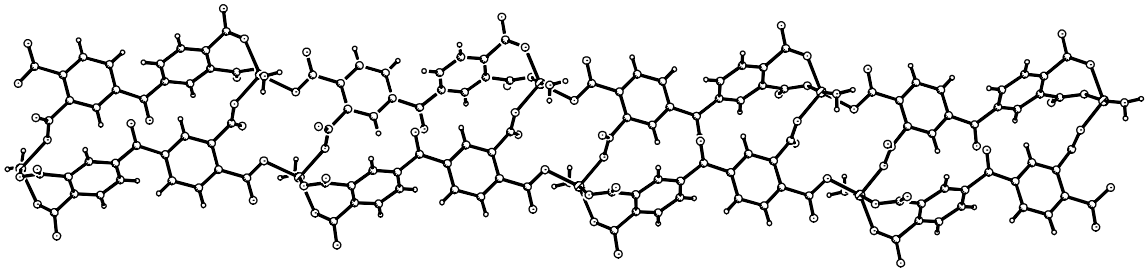

**Figure 2.** Perspective view of the one-dimensional double chain in $\{[Zn(H_2O)_6][Zn(bbtc)H_2O] \cdot 4H_2O\}_n$.

## EXPERIMENTAL

An acetone solution (6 ml) of 3,3′,4,4′-benzophenonetetracarboxylic acid dianhydride (0.2 g) was layered on an aqueous solution (4 ml) of $Zn(OAc)_2$ (0.2 g) in a long test tube. This was sealed with a cork stopper and colorless plate-like crystals deposited after 3 weeks. Anal. Found: C, 29.54; H, 4.22. Calc. for $C_{17}H_{28}O_{20}Zn_2$: C, 29.89; H, 4.13%. Data collection was performed at 293(2) K on a Bruker AXS SMART CCD diffractometer for a colorless crystal $0.12 \times 0.35 \times 0.45$ mm$^3$. $C_{17}H_{28}O_{20}Zn_2$, $M_r = 683.13$, triclinic, space group $P\bar{1}$, $a = 10.585(1)$, $b = 11.518(1)$, $c = 12.306(2)$ Å, $\alpha = 74.194(2)$, $\beta = 66.054(2)$, $\gamma = 73.692(2)°$, $V = 1294.5(3)$ Å$^3$, $Z = 2$, $D_x = 1.753$ g cm$^{-3}$. The structure was solved by direct methods and refined on $F^2$ giving $R_1 = 0.038$ for 406 parameters and 5534 unique reflections with $I > 2\sigma(I)$; $wR_2 = 0.114$ (all data). Programs used: SHELXS-97, SHELXL-97 and ORTEP. CCDC reference number: CCDC 216264.

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